DEVELOPMENT OF OPERATOR TRAINING SIMULATOR USING ASPEN SIMULATION WORKBOOK (ASW): A REACTOR CASE STUDY

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ABSTRACT

Operating Training Simulator (OTS) is a computer-based training system. The OTS applies a simulation of an industrial process to generate the appropriate data of the plant's process operation. In addition, the OTS is widely accepted in the industry as an enabling technology for employee competency and proficiency training and enhancement. This system is deemed as the effective application in order to develop the highest skill levels and proficiency of the operator. This project presents the first-hand experience of developing a process simulator system using Aspen Simulation Workbook (ASW). The production of acetic acid from methanol carbonylation is used as a case study. Aspen Plus is used for the modelling of the methanol carbonylation process and will be linked with Excel using Aspen Simulation Workbook. The simulation can be operated in Aspen Simulation Workbook by manipulating the value of the variables. This case study is about to determine the changes of output variable by manipulates the input variables. This would contribute towards the solution of training issues related to control and operate a process and act as a tool to educate and train the engineering students for supporting training in control and operate certain processes respectively. The operator training tool is developed successfully in Aspen Simulation Workbook.

ABSTRAK

Operasi Simulator (OTS) merupakan satu sistem latihan yang berasaskan komputer. OTS telah mengaplikasikan proses simulasi perindustrian untuk menghasilkan data yang sesuai bagi operasi proses sesebuah kilang. Disamping itu, OTS telah diterima pakai secara meluas dalam industri sebagai satu teknologi yang boleh meningkatkan kecekapan dan latihan kemahiran untuk para pekerja dan kecekapan operator. Sistem ini disifatkan sebagai satu aplikasi yang berkesan dalam usaha untuk membangunkan tahap kemahiran tertinggi dan kemahiran pengendali. Kertas kerja ini membentangkan pengalaman dalam membagunkan proses simulator sistem, dengan menggunakan Aspen Simulasi Buku Kerja (ASW) untuk pengeluaran asid asetik dari methanol carbonylation. Aspen Plus dan dinamik digunakan untuk membangunkan model reaktor yang berkeadaan tetap bagi menghubungkan dengan Microsoft Excel menggunakan Aspen Simulasi Buku Kerja. Ini akan menyediakan integrasi lancar antara model simulasi proses Aspen Tech dan alat kejuruteraan lain dengan lembaran kerja Microsoft Excel tanpa memerlukan pengaturcaraan dan ini juga memudahkan pengguna lain yang tiada pengalaman berkaitan proses simulasi memanipulasi Simulasi Aspen Plus yang kompleks dari Excel. Simulasi ini boleh beroperasi dalam Aspen Simulasi Buku Kerja dengan memanipulasi nilai pembolehubah. Kajian ini adalah untuk menentukan perubahan output berubah dengan memanipulasi pembolehubah input. Ini akan menyumbang kepada penyelesaian isu-isu yang berkaitan dengan latihan mengawal dan mengendalikan proses dan bertindak sebagai alat untuk mendidik dan melatih pelajar-pelajar kejuruteraan untuk menyokong latihan dalam mengawal dan mengendalikan proses tertentu masing-masing. Alat latihan pengendali dibangunkan dengan jayanya di Aspen Simulasi Buku Kerja..

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LIST OF ABBREVIATIONS

OTS	Operator Training Simulator
ASW	Aspen Simulation Workbook
SHE	Process Safety, Health and Environmental
APC	Advance Process Control
CAPD	Computer-aided process design
UK	United Kingdom
USA	United State of America
DCU	Delayed Coker Unit
T	Temperature
P	Pressure
CH_3COOH	Acetic Acid
H_2O	Water
CO	Carbon Monoxide
CH_3OH	Methanol
CO_2	Carbon Dioxide
H_2	Hydrogen
GUI	Graphic User Interface

1 INTRODUCTION

1.1 Motivation and statement of problem

Correct and efficient process operation is becoming increasingly important in the chemical industry as safety requirements and environmental specifications are getting stricter (A.L.Ahmad et al., 2010). 'Safety First' is a tagline that commonly found in almost workplace throughout the world. A numbers of safety policies and standardizations are in place to govern the compliance of safety practice in the workplace (Preston et al.,, 1996). It is well recognized and accepted that safety issue is the most important aspect of industry process operations (Ming et al.,, 2003). Basically, the competency of the operator is really essential to guarantee safety in a workplace. Thus, current employee and operators continually seeks way to improve and increase the competency and performance of its workforce since many workplaces especially chemical plants become more automated (A.L.Ahmad et al., 2010).

The technological development during the last ten years has made simulators for training the engineers and operators in receiving hands-on training ahead of the plant operation, and due to this purpose OTS is considered a necessity in the development of the entire industry (ION, 2010). Adoption of training simulators has been widely practiced in industries where capital investment is high, processes with high complexities and enormous hazardous consequences in case of failure and the industries are not limited to chemical processes, but are also apparent in aviation, shipping, power and energy industry, medical and nuclear system (Cameron et al., 2002, Yang et al., 2001, Murugappan, 2009, Merritt, 2006, Seccombe, 2008).

In the chemical industry, especially in the case of processes, operator training simulators (OTS) are becoming widely used. Operating training simulators (OTS) are computer-based training system for developing and maintaining operational skills in a variety of technical systems (Mani et al.,1990; Kobashi et al., 1995; Okapuu-von Veh et al.,1996; Dudley et al.,2008; Balaton et al., 2013; Manca et al.,2013). With the help of these systems several operations and safety issues can be analyzed, and the operating staff of the plant can be trained in handling different plant failures (Fürcht, Kovács, & Rabi, 2008; Rey, Thiabaud, & Tourdjman, 2008; Yang, Yang, & He, 2001).

Recently, many chemical companies have decided to use OTS system as a tool for training operating staff, rarely used modes of operation and measuring their skills, as well as supporting engineering tasks like testing new methods and performing safety test without risk on the real system. To fully accomplish the OTS successfully, a structured model of high computational complexity comprising a large number of state variables and parameters. Several often difficult to measure or determine, is required. However, for computational reasons the OTS model should preferably be kept as simple as possible. The main part of the OTS is the process model that replaces the real technology and an OTS is an example of high fidelity simulation model application. These models are mathematical representations of actual plants that accurately mimic the process conditions on the plant using chemical engineering theory (Jago, 2008).

Training, or person's readiness, is perhaps the most important aspect of the success of operational readiness. An untrained operator is not competent to run the plant to the optimum degree of efficiency. Taking an analogy to autopilot, advanced process control (APC) typically removes the reactive actions required by a process operator to allow more time to be spent on optimizing production. However, from time to time, operators need to be able to take control of the process to manage an upset. This gap can be filled by an OTS, analogous to a flight simulator, it is proved to be extremely valuable, allowing the operator to continually develop skills, make mistakes and learn in a safe simulated environment (ARC, 2009, Merritt, 2006, Murugappan, 2009). For ensuring the effectiveness of an OTS, its backbone, the models need to be rigorous and robust enough to cover all the operations. These high fidelity models need to represent key operating scenarios such as start-up, shutdown, normal operations and also abnormal situations, such as equipment failure (Mhammed, 2005) (Muravyev A. a., 2007). This feature is inarguably the most important and vital element for a good and reliable simulator.

OTS system also can be used in an educational sector as a tool to educate and train the operators for supporting training in control and operate certain processes. Pre-training in the OTS environment prior to practical training in the plant or laboratory environment could significantly enhance the efficiency of learning of the process operators. In particular, the operators' understanding of the complexity of the process, ability to make correct operational decision and adhere to standard routines could be expected to be improved (Lee, 2005). So far, few efforts have been made to exploit the potential of OTS for supporting training in process manufacturing. Especially, production processes may benefit substantially by using OST due to their inherent complexity, complicated operational procedures and wide-spread use in large-scale industrial production.

Computer-aided process design (CAPD) and simulation tools have been successfully used in industries since the early 1960s for the development and optimization systems. Simulators used in these industries are designed to simulate processes and their behavior, mainly for process control purposes. From the available simulators, Aspen Plus (Aspen Technology,Inc.), HYSYS (Aspen Technology,Inc),and PRO/II (Simulation Sciences,INC.) are the most widely used. In OTS applications, the entire plant is to be simulated. However, the simulation of the auxiliary units might be more difficult. The most advantageous solution would be the connection of these software programs. Numerous studies have been conducted to elucidate the functions and benefits of operator training simulator (OTS) in the industry. Although the function of OTS is well understood, however, no research has been performed for developing an operator training simulator by using Aspen Simulation Workbook (ASW), and therefore this is the aim of this study.

ASW enable seamless interoperability between AspenTech's engineering tools and Microsoft Excel with no programming required. ASW is a powerful tool that allows Aspen Plus and Aspen HYSIS simulation experts to easily create a clean user interface for their models in Microsoft Excel. This makes it easy for other users to manipulate complex Aspen Plus simulations without being intimately familiar with the models or even the software used. It brings the power of process modelling to a wider range of users, allowing us to expand the use of process models to solve plant operating problems (Aspen Technology,Inc, 2014). The main objective of this study was to develop operator training simulator using Aspen Simulation workbook for reactor case study and the production of Acetic acid via methanol carbonylation process was chosen as a case study for this project.

1.2 Objectives

The following are the objective of this research:

- To develop an operator training simulator by using Aspen Simulation Workbook (ASW) for a production of acetic acid process.

1.3 Scope of this research

The following are the scope of this research:

i) **Develop a reactor model** to produce acetic acid via a methanol carbonylation process by using Aspen PLUS.

ii) **Develop GUI and Embedding the simulation** case files using Aspen Simulation Workbook (ASW) in Microsoft Excel.

iii) **Test the Operator Training Simulator (OTS)** by running scenarios of case study.

1.4 Main contribution of this work

The following are the contributions

i) Solution of training issues related to control and operate a chemical process.

ii) Tools to educate and train the engineering students or inexperienced operators for supporting training in control system changes and test those changes against the simulator.

1.5 *Organisation of this thesis*

The structure of the reminder of the thesis is outlined as follow:

Chapter 2 provides a summary of the literature of Operator Training Simulator (OTS) in worldwide company and the previous work on the production of acetic acid process by methanol carbonylation. General descriptions of the flow characteristic of the system, as well as the information on reaction are presented. This chapter also provides a brief description of the reactor operating conditions, including the type of the reactor, the temperature, and also the pressure of the reactor used. A brief description of the simulation software is also provided.

Chapter 3 gives a review of the methodology for the development of Operator Training Simulator using Aspen Simulation Workbook for acetic acid production. This chapter discuss on the developing simulation model by using Aspen Plus and also the steps to connect the simulation model with the Excel by using Aspen Simulation Workbook.

Chapter 4 discuss about the result of the case study of acetic acid production. The model is developed using Aspen Plus simulation software based on the data from previous kinetic modelling. The reactants used are methanol, carbon monoxide and water and the main product of the process is acetic acid.

Chapter 5 is about the conclusion from the objectives of the experiment and some recommendations to improve our skills in simulator training.

2 LITERATURE REVIEW

2.1 Overview

This paper presents the development of Operator Training Simulator (OTS) using Aspen Simulation Workbook for the production of Acetic Acid by methanol carbonylation case study. The technological development during the last ten years has produced simulators as a tool for training engineers and operators in receiving realistic hand-on training ahead of the plant start-up and throughout plant operation. Due to this purpose, the simulator has been considered a necessity in the development of the entire industry since correct and efficient process operation becoming increasingly important in the chemical industry as safety requirements and environmental specification is getting stricter. The simulation model was done using Aspen Plus. Then, the integration between the simulation model with Microsoft Excel is provided by Aspen Simulation Workbook (ASW). Then, the ASW will allow modelling experts to link model and plant data and publish the resulting model as Excel worksheet.

2.2 Recent Development of Operator Training System in Industry

The first Operator Training System was developed and launched in MOL's Danube Refinery at Százhalombatta in the Delayed Coker Unit (DCU), paralelly to unit start-up in 2001. The advanced technical state of the Danube Refinery and the further developments generated extended demand for skilled and well-educated employees. In order to meet this demand, the Refinery management decided to upgrade the existing OTS in the Delayed Coker unit and to implement new systems for the most important units. After the project definition period the OTS Project started at the Danube Refinery in 2005. Based on the results further steps are planned: more Training Systems will be implemented in the 2007-2010 timeframe. (ákos Fürcht, kovács, & rabi, 2008).

The purpose of simulations is that by simulating a process the engineers can follow and view the entire system over time, without having to change, interrupt and affect it. It is important to remember that the decision they make and the actions they take can have a deep impact on the project success indicators involving areas related to cost, risk, quality and schedule. The dynamics of complex processes are not exact replicas of the real system dynamics, but it is an approximation that makes the relationships between different parts of the system possible to understand (Ferreira et al., 2012). On the market today there are different tools available for both dynamic and steady state simulations. Ideally, it should be easy to switch between the two simulations and therefore it is important that the two models can be simulated in the same tool without changing the environment. In order to include both experienced and non-experienced engineers and operators, it is important that the simulator is easy to use (Bezzo et al., 2004).

In the chemical field, KBR has an outstanding team of technology, simulation and training experts who help translate our business goals of safe, economic and reliable operation into tailored solutions for our facility. The KBR, Inc (Kellog Brown & Root) are an American engineering, construction and private military contracting company which is a worldwide company that include the Americas, Africa, Asia-Pacific, Australia, Europe and the Middle East .(KBR, 2013)

An Operator Training Tool System (OTS) is the only tool that ensures plant operators receive plant specific and realistic hands-on training ahead of plant start-up and throughout plant operation. KBR's user-friendly OTS systems are configured with KBR’s proprietary reactor models and physical property methods and include scenarios that are particular to our specific plant and process. As a complement to classroom training, a comprehensive portfolio of training scenarios allows operators to reach competency in a safe, realistic, repeatable and hands-on environment. (KBR, 2013)

Benefits of OTS Include:

i. A typical 30% reduction in the training time of an experienced workforce
ii. For a non-experienced workforce, training times drop from one-three years to six months
iii. A three-five day reduction in the initial start-up time of a typical process plant
iv. Confidence knowing that plant automation systems are fully tested prior to start up

Long Term Benefits of OTS Include:

i. Operational best practices are reinforced through refresher training
ii. Increases workforce flexibility through cross-trained operators
iii. The opportunity to test trial modifications to the plant's control and automation systems and process configurations
iv. The development and refinement of operating procedures
v. OTS training helps accelerate Advanced Process Controls (APC) implementation

KBR enhance the value of OTS systems by deploying integrated engineering, commissioning and simulator teams on projects. In this way the user is able to drive synergies between and across projects that deliver increased benefits to our customers. (KBR, 2013)

2.3 Feature of an Operator Training Simulator

This OTS is used for training in both the process behavior of the plant as well as the use of distributed control system (DCS) to control the plant. As actual hardware of a DCS is very costly, a very good emulation of DCS graphics and control outlook was adopted. Figure 2-1 shows the analogy of OTS to real plant. The plant dynamic model and the actual process plant were analogous. The instructor station could be considered an analogy to the control system in real plant, where it invokes responses from operator through the operator control console. The operator console or DCS of actual plant is analogous to the emulated operator consoles.

Besides training for plant start-up, shutdown and normal operation, OTS training also covers emergency situation handling. Through instructor station, various possible condition could be initiated. A few examples were the cold start up, hot startup, emergency shutdown and malfunctions such as pump tripping.

Training would be more meaningful and effective if evaluation could be carried out. Hence, OTS does include evaluation function for tracking of operating procedures and actions in order to measure a trainee's performance. The instructor could define the acceptable operating ranges and specified a time frame for process recovery as the basis for the evaluation.

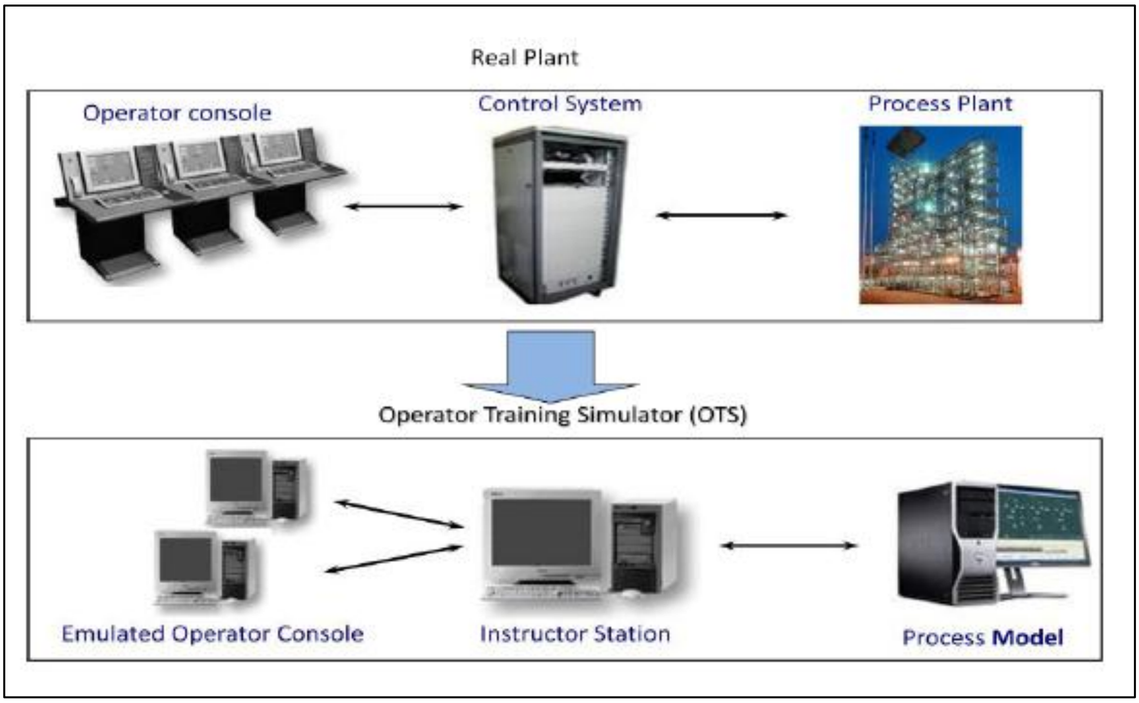

Figure 0-1: Operator Training Simulator System in Industry

The Figure 2-1 was showed the operator training simulator system in industry which is OTS solution is a cost effective high-fidelity simulated operator training solution that realistically resembles the operator station appearance and functionality, while at the same time, increases the training capabilities and flexibility of the system. The OTS will offer a highly realistic representation of plant operation and will provide a unique environment for developing operation skills and studying detailed process behaviour, using customized simulation models. Various operational conditions will be provided for the simulated plant, including start-up, shutdown, emergency conditions and normal operational transients.

2.4 Previous work on Production of Acetic Acid from Methanol Carbonylation

Acetic acid has been very familiar to mankind since it has been used as vinegar for a long time and the demand of acetic acid is about 5.4 million tons/year in the world in 1997. Acetic acid is used in vinyl acetate, solvent for the production of pure terephthalic acid (PTA), acetic anhydride, acetates, and others. In the mean time, the manufacturing process of acetic acid by the carbonylation of methanol was developed. This process uses methanol and carbon monoxide as raw materials which are produced from natural gas, coal, heavy residual oil, and others. BASF (Germany) industrialized this process in 1960, and Monsanto (USA) industrialized it in 1970. Especially the latter process, known as Monsanto process, has become the dominant industrial route for acetic acid manufacturing.

This methanol carbonylation, which is also called as Monsanto process, uses methanol and carbon monoxide as the raw materials to synthesize acetic acid. Because the price of naphtha has risen and the relatively cheap methanol, produced from off gas, natural gas, and so on, has been available after the oil crisis, this process has rapidly become prevalent. At present, this process accounts for 60% of the production capacity of the world. The overall stoichiometry of the acetic acid synthesis is represented simply by

$$CH3OH + CO \rightarrow CH3COOH$$

In the Monsanto process, the selectivities to acetic acid based on methanol and carbon monoxide are 99% and 90%, respectively, when rhodium is used as a catalyst and iodine as an activator. These days, most of the methanol carbonylation process has adopted this catalyst system (Ken-ichi Sano., Hiroshi Uchida., Syoichiru Wakabashi, 1999).

The flowsheet of methanol carbonylation process was shown in Figure 2-2. Methanol and carbon monoxide are supplied continuously into the reactor. The exhaust gas from the reaction section, together with exhaust gas from the purification section, is washed in the scrubber, then the light-ends are recovered and recycled to the reaction section. On the other hand, the reaction product (crude acetic acid) is sent to the light-ends column, and acetic acid is taken out as a side-cut. The overhead and the bottoms including the catalyst return to the reaction section. Side-cut acetic acid is sent to the dehydration column, then the mixture of water and acetic acid is taken out from the top, and returned to the reaction section. The bottoms of the dehydration column are sent to the subsequent product column. A small amount of the heavy-ends,which contain propionic acid, is taken out from its bottom.The overhead is further purified in the next fractionation column, and purified acetic acid is obtained as a side-cut.The overhead and the bottoms of the fractionation column are recycled into the reaction section.

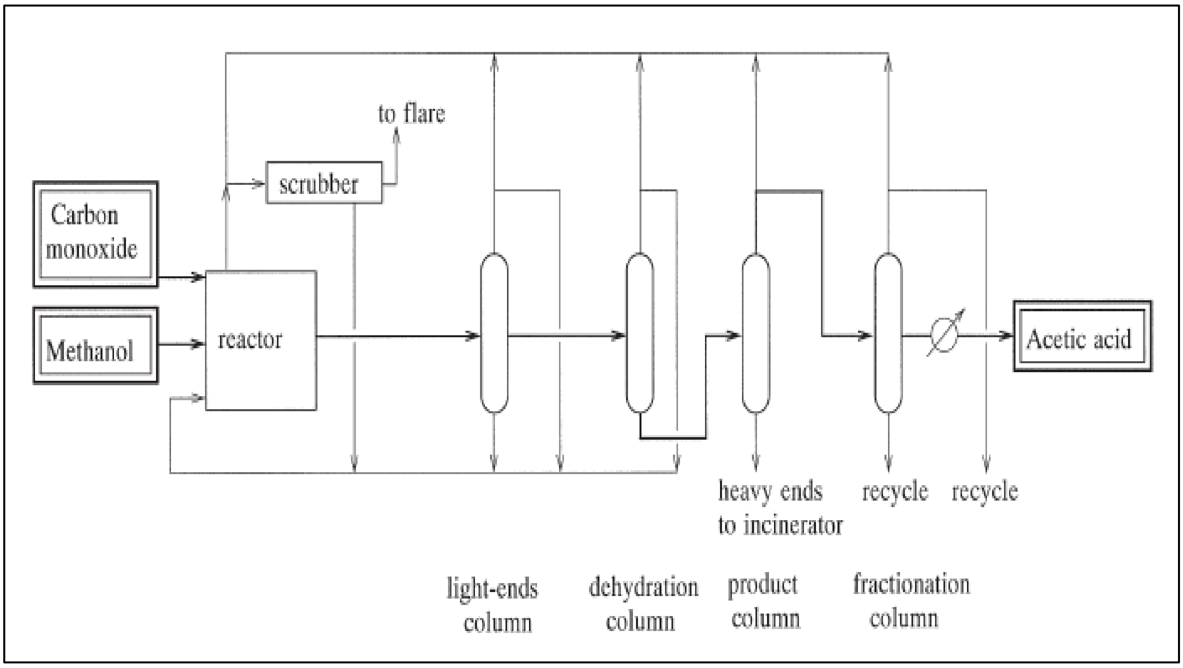

Figure 0-2: Process flowsheet of methanol carbonylation process

2.5 Simulation for develop model

In this research, the software that were used to develop an operator training tools is Aspen Simulation Workbook whereas the steady-state simulation was done using Aspen Plus. Aspen Plus is a comprehensive chemical process modelling system, used by the world's leading chemical and specialty chemical organizations, and related industry to design and improve their process plants. In addition, Aspen Plus also takes a steady - state process modelling to the next level, allowing to create powerful dynamic simulation for better analysis of plant behavior and safety.

Aspen Simulation Workbook is one of the sub-programme from the AspenTech. Aspen Simulation Workbook enables integration between AspenTech's simulators, such as Aspen Plus and Aspen HYSYS, and Microsoft Excel. For plant operations, Aspen Simulation Workbook accelerates the adoption of process models for operations decision support, bringing the power of simulation to non-simulation experts (Aspen Technology, 2004).

Aspen Simulation Workbook (ASW) is a tool for interfacing AspenTech's process simulation models with Microsoft Excel worksheets. Aspen Simulation Workbook also has tools to link model variables to plant data tags imported using third-party applications. These capabilities allow modelling experts to link models and plant data and publish the resulting models as Excel worksheets for use by casual model users(Aspen Technology, 2004).

2.6 Summary

This paper presents how an Operator Training Simulator (OTS) works in industry. Nowadays, the companies would like to operate the plant using systems because they know the benefits from the technology will contribute more to the company. Instead of the system is low cost, it also care for environment surrounding to improve safety and increase their overall profitability, always cognizant of environmental impact.

3 SIMULATION METHODOLOGY

3.1 Overview

This paper presents the development of Operator Training Simulator (OTS) by using Aspen Simulation Workbook (ASW) and solve the problem of the reactor case study . ASW provides seamless integration between AspenTech's engineering tools and Microsoft Excel, allowing us to deploy models to a wider range of users. The result is new levels of value to improve productivity during conceptual design and the expanded use of process models in operations for performance monitoring, better decisions, and optimization. Therefore, ASW is a powerful tool for creating convenient user interfaces to Aspen Plus model in Microsoft Excel. It brings the power of process modeling to a wider range of users, allowing us to expand the use of process models to solve plant operating problems such as equipment troubleshooting, performance improvement and other plant studies, driving greater value from my simulation investment. This makes it easy for other users without process simulation experiences to manipulate complex Aspen Plus simulation from Excel (Leviene & Tremblay, 2012). In this study, the reactor model was designed and developed by using Aspen Plus. Then, the graphic user interface (GUI) of the OTS was developed and embedded in Microsoft Excel by using Aspen Simulation Workbook (ASW). Lastly, the scenarios of the case study were run to determine the changes of the output variables by manipulating the input variables of the reactor.

3.2 Process Modelling

Process modelling is done by using process simulators. Although it was far from reality, the process simulators were designed to simulate processes and their behaviour, mainly for process control purposes. In other word, process simulators are used to mimic the real processes. Equipped with advance computation techniques, comprehensive thermodynamic packages and large component libraries, process simulators today provides reliable information of process design and operations. In this work, the case was modelled using Aspen Plus. The important steps to process modelling and simulation using process simulators include defining the chemical components, selecting the thermodynamic model and method, designing the process flow sheet by choosing proper operating units, determining plant capacity and setting up input parameters.

The steady state simulation model for methanol carbonylation process was carried out using Aspen Plus Simulation. The important steps to develop the simulation model was shown in Figure 3-1. In defining the process flow sheet, it is very important to define the unit operation and streams that's flowing to and from the unit operational in the process. Aspen Plus is a steady state chemical process simulator. It used unit operation blocks, which are models of specific process operation (reactors, heaters, pumps, distillation column, etc.). Then, these blocks were placed on a flow sheet, specifying material and energy streams. The model was selected from the Aspen Plus Model Library to describe each unit operation. Then, the labelled streams were placed on the process flow sheet and connected to the unit operation model to complete the steps. Then, the labelled streams were placed on the process flow sheet and connected to the unit operation model to complete the steps. Then, the chemical components in the process were specified. In this case, the chemical components that were specified are Methanol, Carbon Monoxide, Water, Hydrogen, Carbon Dioxide and Acetic Acid. All the chemical components were taken from the Aspen Plus databanks. Then, the thermodynamic model was specified to represent the physical properties of the components and mixtures in the process.

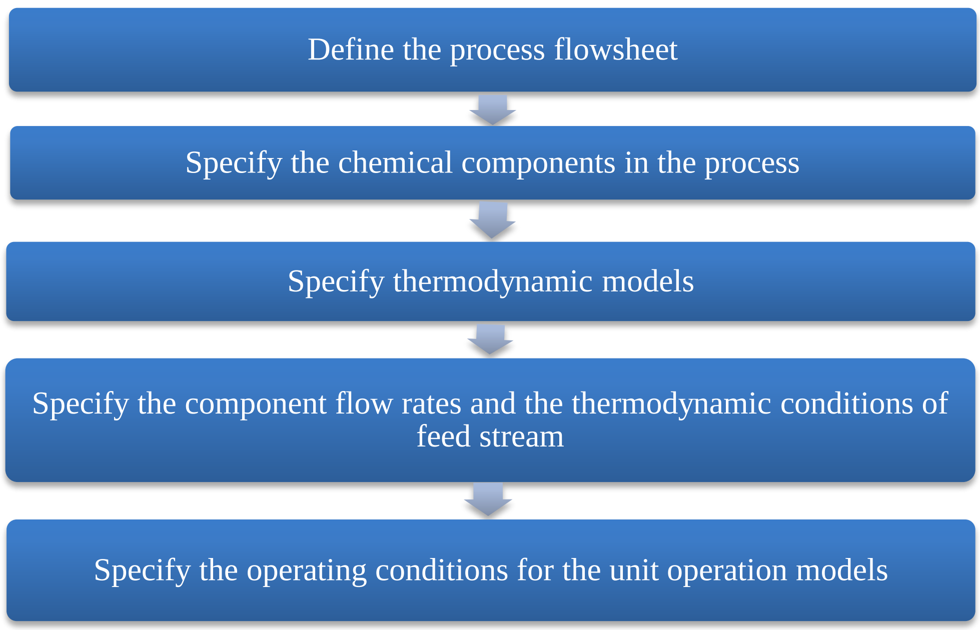

Figure 3-1: Steps in developing simulation models in Aspen Plus

3.3 Designing a Model of Methanol Carbonylation Process in Aspen Plus

The designed process flow diagram of acetic acid production via methanol carbonylation in Aspen Plus was shown in Figure 3-2 . It consists of the equipment and streams. The equipment selection is very important in order to meet the demand of the acetic acid production with high purity while minimized the cost of equipment used. This process was used the NRTL thermodynamic model and method because the components used were in the vapor and liquid phase (Job Lindenbergh, 1996).

In this case, the component compounds used in the simulation work are methanol, carbon monoxide, water, acetic acid, carbon dioxide and hydrogen. The raw materials used are methanol, carbon monoxide and water with mass fraction (w=1) respectively, whereas the output product from the process are acetic acid, carbon dioxide and hydrogen. The reaction section exists at a reactor (R-100), in which methanol was carbonylated with carbon monoxide and water to produce acetic acid with carbon dioxide and hydrogen gas as byproducts, and a distillation column (D-100) as purification of the product.

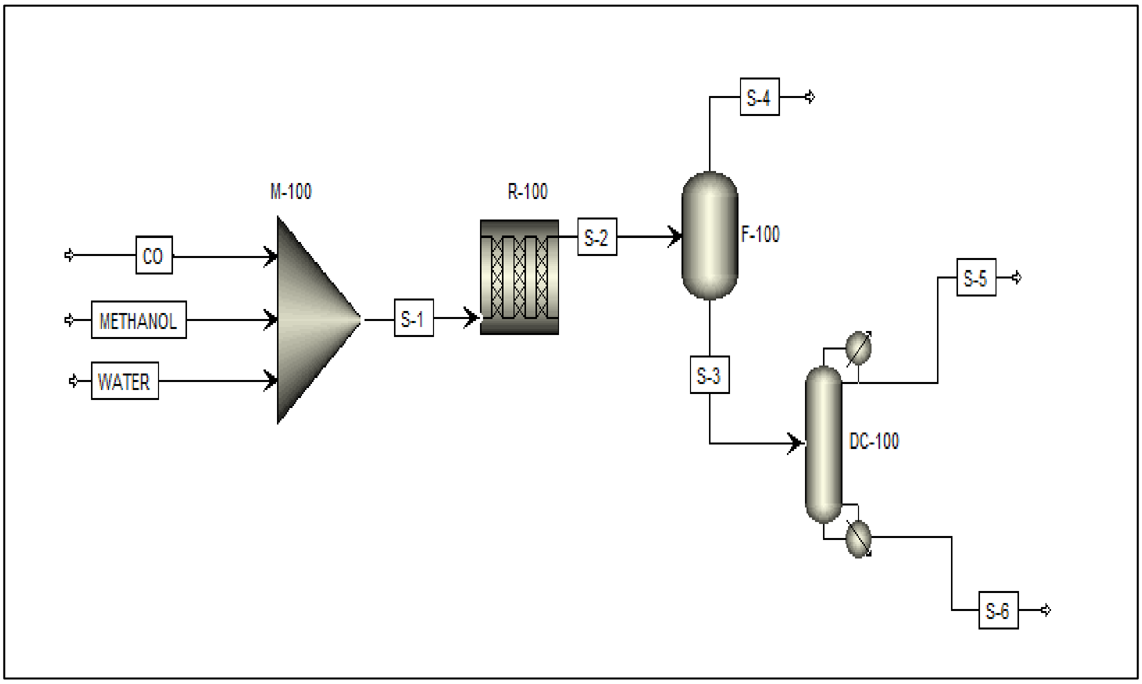

Figure 3-2: Simulation Model for Methanol Carbonylation Process

The equipments used in this model are mixer, plug flow reactor (R-Plug), flash distillation drum, and distillation columns (DSTWU). The operating conditions were set for methanol and carbon monoxide in gas phase 175 ^{o}C and 36 bar while for water in liquid phase is heating up at 80 ^{O}C and 36 bars (Job Lindenbergh et al.,, 1996). Every inlet feed mixtures must occur at a slightly higher pressure than our operating reactor condition to prevent backflow of feed mixtures to the mixer (Suzuki, I.Y, 1971). The properties of the materials involved in the process are given in Table 3-1.

Material	**Formula**	**Molecular Weight (g/mol)**	**Melting Point (℃)**	**Boiling Point (℃)**	**Density (kg/l)(20℃)**
Methanol	CH_3OH	32.04	-97.6	64.7	791.8
Carbon Monoxide	CO	28.0	-205	-191	0.001
Acetic Acid	CH_3COOH	60.1	17	118	1.049
Carbon Dioxide	CO_2	44.0	n.a	-79	0.001
Water	H_2O	18.0	0	100	1.000
Hydrogen	H_2	2.0	-259	-253	0.089

Table 3-1: Materials involved in the process (Job Lindenbergh, 1996)

3.4 The Reaction Kinetics of Methanol Carbonylation

The overall reaction in the reactor for the acetic acid synthesis via methanol carbonylation is represented simply by

$$2\ CO + H_2O + CH_3OH \rightarrow CH_3COOH + CO_2 + H_2$$

In aqueous media the rate is found to be dependent on carbon monoxide and methanol concentrations. However, with respect to a carbon monoxide concentration the rate is first order at low partial pressures of carbon monoxide and zero order at high partial pressure (above 3 bar) (Howard, 1993). In acetic acid media the rate shows a zero-order